

The development and application of thermodynamic and atomic mobility databases for Cu-based alloys

Ying Tang and Qing Chen

Thermo-Calc Software AB, SE-113 64 Stockholm, Sweden

A thermodynamic database (TCCU) and an atomic mobility database (MOBCU) for copper alloys, including 27 elements, have been developed. Both the thermodynamic and mobility databases are obtained through a hybrid approach of experiments, first-principles calculations, and CALPHAD approach. The present thermodynamic database can be used to calculate various phase diagrams and property diagrams in the assessed systems or even extrapolated higher-order systems. It will help to understand the phase equilibria in multi-component industrial copper alloys and can be used to predict the phase formation, phase fractions, and phase compositions or to calculate the driving force of a phase transformation. Besides, by coupling the present mobility database with thermodynamic database, various diffusivities in both solid and liquid solution phases in Cu-based alloys can be calculated. Furthermore, they can be applied to simulate diffusion-controlled phenomena, such as solidification, nucleation, growth / dissolution and coarsening of precipitates by using DICTRA or TC-PRISMA.

Typical examples of various calculations and application of these two databases to different copper alloys are presented. These newly developed databases are expected to be continuously improved and extended in future and will provide fundamental thermodynamic and kinetic data for computer-aided design of copper base alloys.